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CFD Analysis of Hydrogen Leakage from a Small Hole in a Sloping Roof Hydrogen Refueling Station

Weiyi Cui[1, 2, 3], Liang Tong[1, 2, 4] , Yupeng Yuan[1, 2, 4, 5] and Chengqing Yuan[1, 2, 4, 5]

[1] State Key Laboratory of Maritime Technology and Safety, Wuhan University of Technology, Wuhan, 430063, China.

[2] National Engineering Research Center for Water Transport Safety, Wuhan University of Technology, Wuhan, 430063, China.

[3] School of Naval Architecture, Ocean and Energy Power Engineering, Wuhan University of Technology, Wuhan, 430063, China

[4] Reliability Engineering Institute, School of Transportation and Logistics Engineering, Wuhan University of Technology, Wuhan, 430063, China, ypyuan@whut.edu.cn

[5] Academician Workstation of COSCO SHIPPING Group, Shanghai, 200135, China

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OUTLINE

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INTRODUCTION

- Ports are the gathering point and hub of the shipping industry and land transportation, and the lifeline of national economic development. Zhoushan Port in Ningbo of China, as the largest port in terms of container throughput, emits 1.05 million tons of carbon in 2020.
- In order to achieve carbon peaking and carbon neutrality goals, Ningbo Port plans to build a hydrogen refueling station to meet the needs of hydrogen energy equipment in the port area.
- The CFD software FLUENT was used to study the influence of leakage angles on the leakage of high-pressure hydrogen through a small hole.
- Considering the calculation accuracy and efficiency, this paper adopted the pseudo-diameter model.

THEORETICAL MODEL

Mass conservation equation:

$$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x_i}(\rho u_i)=0$$

Momentum equation:

$$\frac{\partial}{\partial t}(\rho u_i)+\frac{\partial}{\partial x_i}(\rho u_i u_j)=-\frac{\partial p}{\partial x_i}+\frac{\partial \mathcal{T}_{ij}}{\partial x_i}+\rho f_i$$

Energy equation:

$$\frac{\partial}{\partial t}(\rho E)+\frac{\partial}{\partial x_i}[u_i(\rho E+p)]$$
$$=\frac{\partial}{\partial x_j}\left[\left(k_{\mathrm{eff}}+\frac{c_p\mu_{\mathrm{t}}}{\mathrm{Pr}_{\mathrm{t}}}\right)\frac{\partial T}{\partial x_j}+u_i(\mathcal{T}_{ij})_{\mathrm{eff}}\right]$$

Species transport equation:

$$\frac{\partial}{\partial t}(\rho w_n)+\nabla\cdot(\rho \boldsymbol{u} w_n)=-\nabla\cdot \boldsymbol{J}_s$$

Turbulence model:

Realize κ-ε turbulence model

The turbulent kinetic energy κ equation:

$$\frac{\partial(\rho\kappa)}{\partial t}+\frac{\partial(\rho\kappa u_j)}{\partial x_j}$$
$$=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_{\mathrm{t}}}{\sigma_\kappa}\right)\frac{\partial \kappa}{\partial x_j}\right]+G_\kappa+G_b+S_\kappa-\rho\varepsilon-Y_M$$

Dissipation rate ε equation:

$$\frac{\partial(\rho\varepsilon)}{\partial t}+\frac{\partial(\rho\varepsilon u_i)}{\partial x_i}$$
$$=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_{\mathrm{t}}}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right]+\rho \mathrm{C}_1 E\varepsilon-\rho\mathrm{C}_2\frac{\varepsilon^2}{\kappa+\sqrt{\nu\varepsilon}}$$
$$+\mathrm{C}_{1\varepsilon}\frac{\varepsilon}{\kappa}\mathrm{C}_{3\varepsilon}G_b+S_\varepsilon$$

Leakage mass flow rate:

$$Q=C_0A_1p_0\sqrt{\frac{M\gamma}{RT_1}\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{\gamma-1}}}$$

THEORETICAL MODEL

Pseudo-diameter model

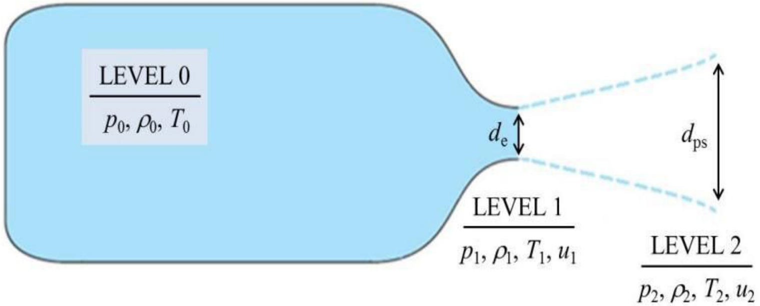
- Birch
- Ewan and Moodie
- Yuceil and Otugen
- Schefer
- Molkov

According to recommendation by Li et al.*, the model proposed by Birch in 1987 is chosen for this simulation.

Birch-1987 Model:

The gas leakage process follows the laws of conservations of mass, momentum and energy.

The temperature and pressure of the gas **are equal to the temperature and pressure of the environment.**



Mass conservation equation:

$$\rho_1 u_1 A_1 = \rho_2 u_2 A_2$$

$$A_1 = \frac{\pi d_e^2}{4}$$

$$A_2 = \frac{\pi d_{ps}^2}{4}$$

Momentum conservation equation:

$$\rho_2 u_2^2 A_2 = \rho_1 u_1^2 A_1 + (p_1 - p_2) A_1$$

Pseudo diameter:

$$\frac{d_{ps}}{d_e} = \frac{\rho_1 u_1}{\sqrt{\rho_{gas}(p_1 - p_\infty + \rho_1 u_1^2)}}$$

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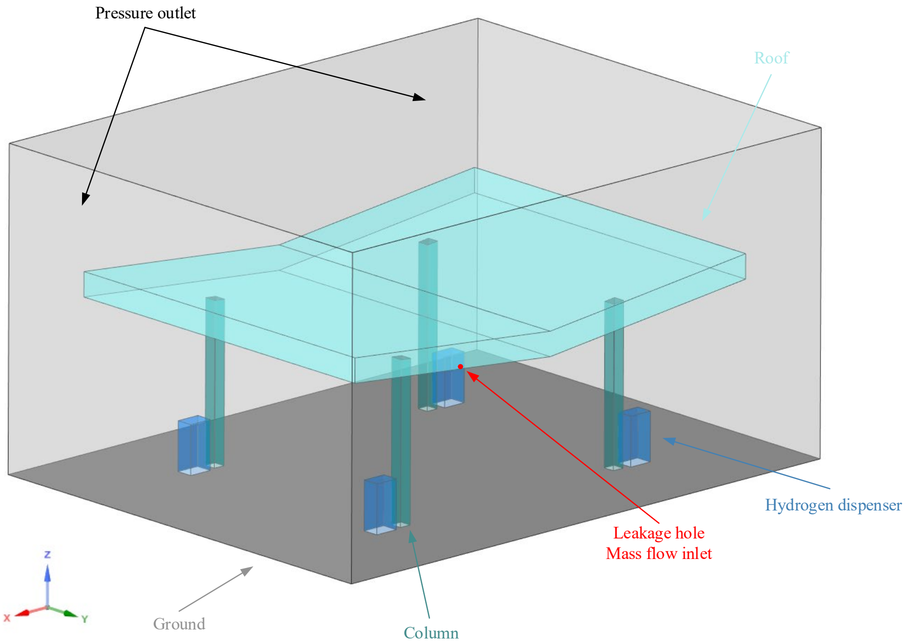
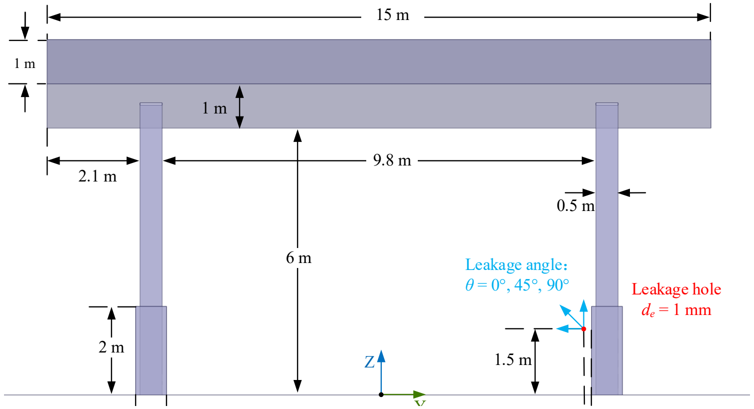
*Li X, Christopher D M, Hecht E S, et al., Comparison of two-layer model for high pressure hydrogen jets with notional nozzle model predictions and experimental data, 6th International Conference on Hydrogen Safety, 19-21 October 2015, Yokohama, Japan.

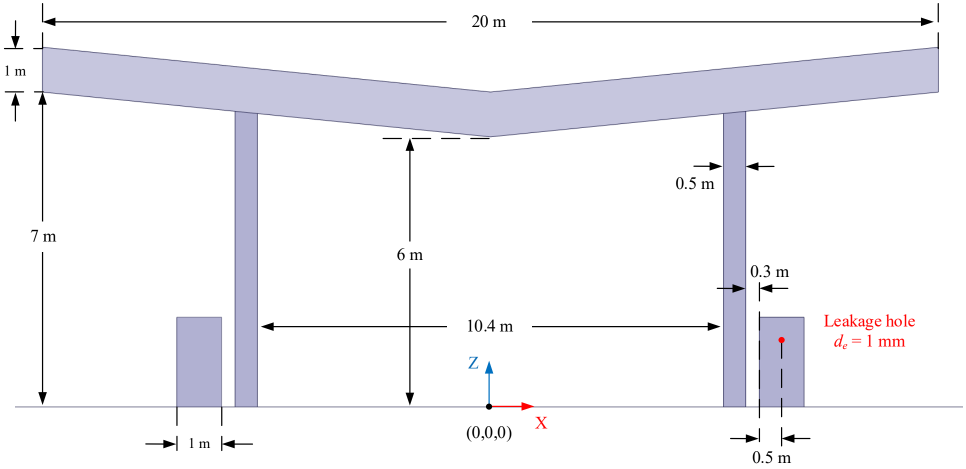
THEORETICAL MODEL

Hydrogen refueling station geometry model

By investigating the historical incidents at hydrogen refueling stations*, it was assumed that the filling hose had **failed to seal due to wear.** d_e=1 mm, d_{ps}=13.06 mm. Leakage hole diameter 1mm







b. XZ section of sloping roof hydrogen refueling station

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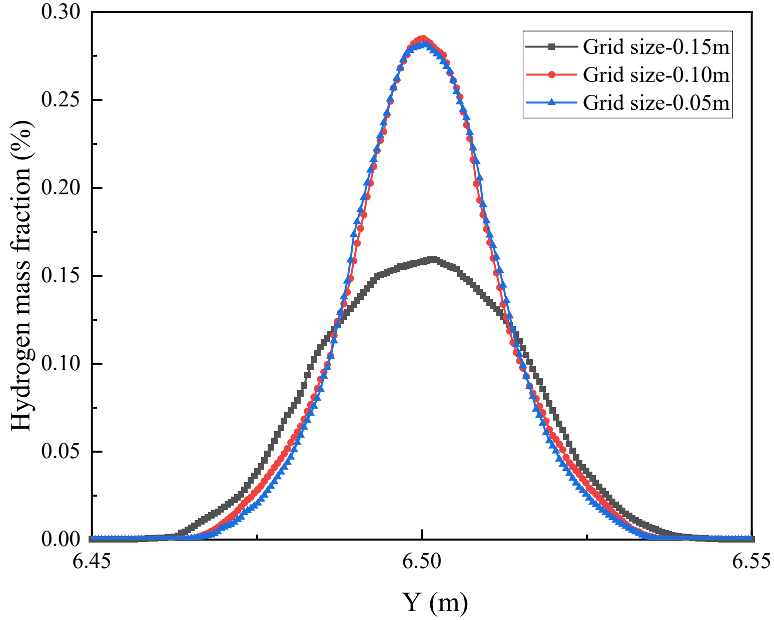
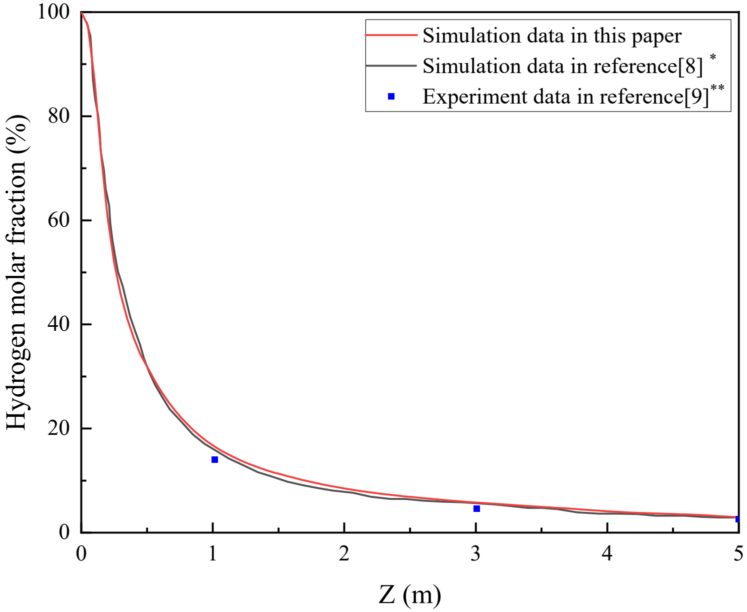
* *Yang F, Wang T, Deng X, et al., Review on hydrogen safety issues: Incident statistics, hydrogen diffusion, and detonation process. International journal of hydrogen energy, 46, No. 61, 2021, pp. 31467-31488.*

** *Sakamoto J, Sato R, Nakayama J, et al., Leakage-type-based analysis of accidents involving hydrogen fueling stations in Japan and USA. International journal of hydrogen energy, 41, No. 46, 2016, pp. 21564-21570.*

THEORETICAL MODEL

CFD model validation





Three meshes with different sizes were created for mesh-independent validation. The results of the two cases with grid numbers 292852 and 458289 did not differ much, while the case with grid number 156983 shows a significant deviation from the remaining two cases. So the case with 292852 grid was chosen.

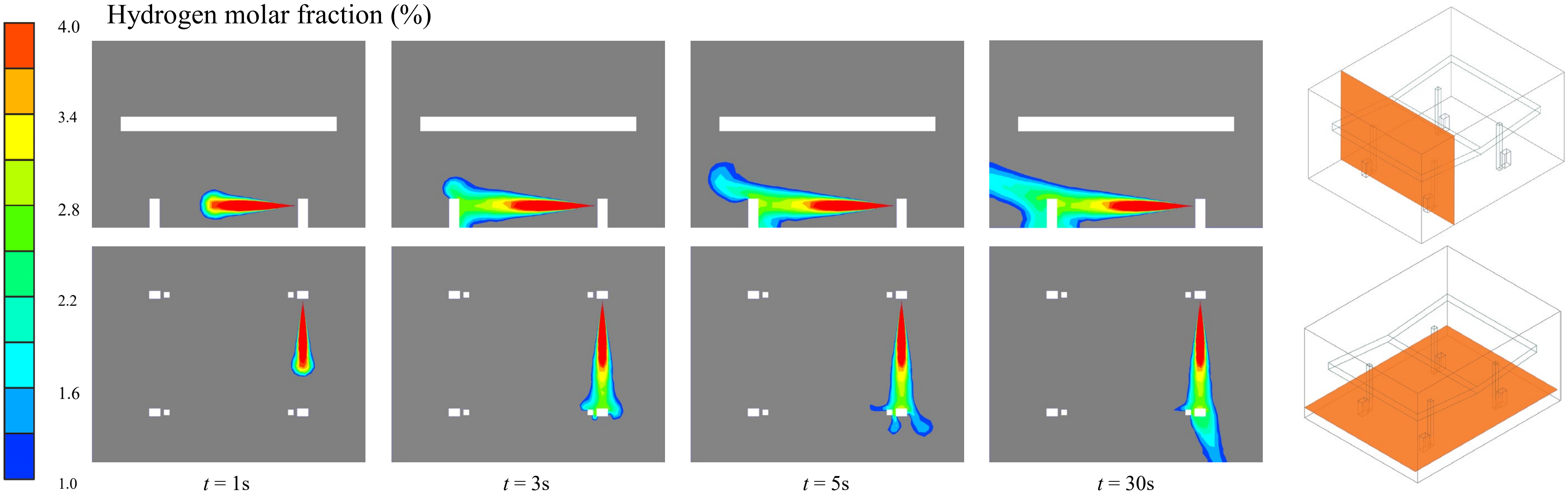
Comparison with experimental and simulation data of other scholars has been carried out to validate the model accuracy. The simulation data in this paper (red line) agreed with the simulation data (black line) and experimental data (blue rectangles).

** Li X, Christopher D M, Hecht E S, et al., Comparison of two-layer model for high pressure hydrogen jets with notional nozzle model predictions and experimental data, 6th International Conference on Hydrogen Safety, 19-21 October 2015, Yokohama, Japan.*

*** Han S H, Chang D, and Kim J S., Experimental investigation of highly pressurized hydrogen release through a small hole. International journal of hydrogen energy, 39, No. 17, 2014, pp. 9552-9561.*

RESULTS AND DISCUSSION

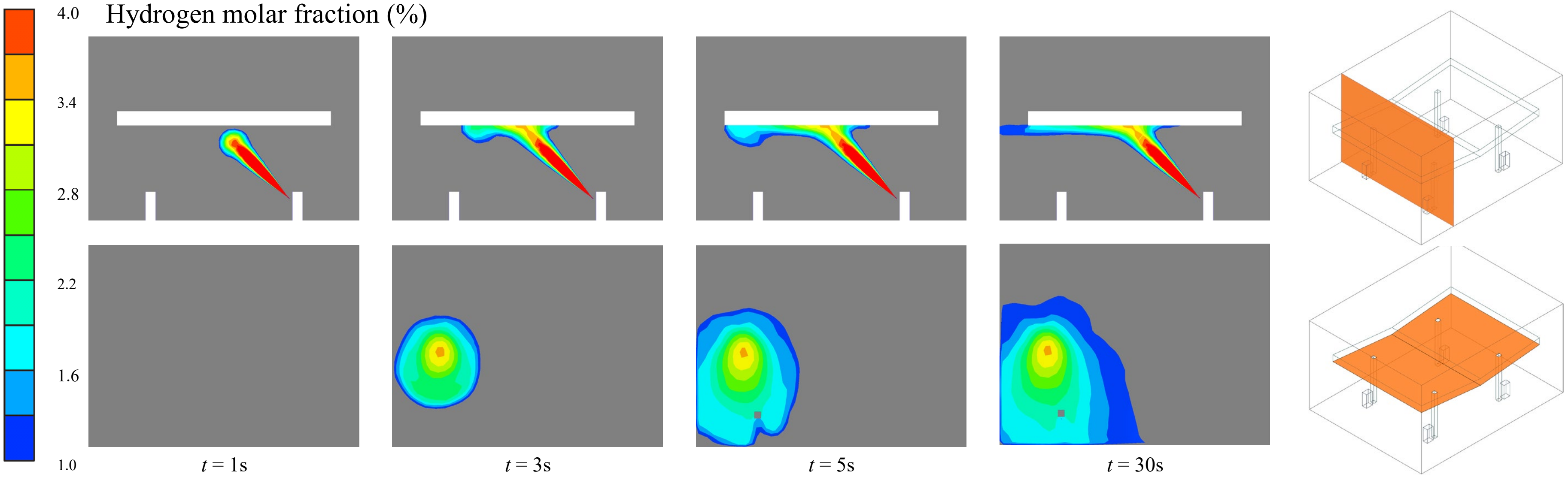
Leakage angle θ=0°



- The momentum of the diluted hydrogen (vol% from 1% to 4%) in the outer layer of the hydrogen jet has **dropped significantly**.
- Large amounts of hydrogen reached stagnation near the obstacle, and the volume of the hazardous hydrogen (vol% above 1%) cloud **kept rising**.

RESULTS AND DISCUSSION

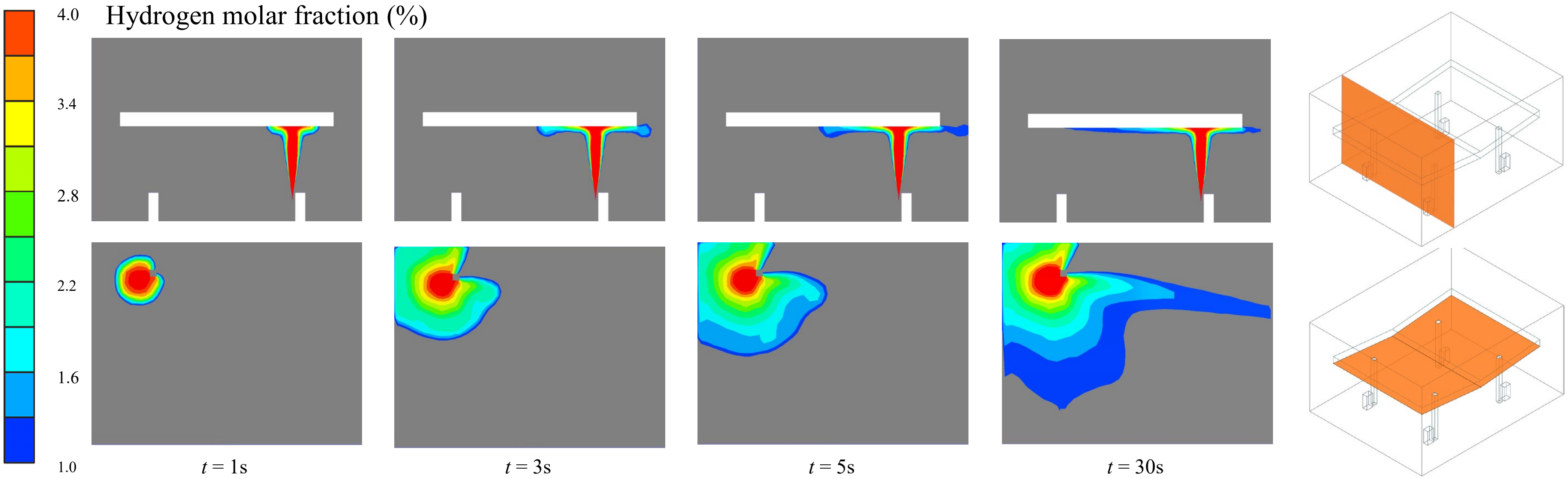
Leakage angle θ=45°



- The hydrogen diffused along the underside of the roof showed a **significant accumulation**.
- Due to the obstacle of the roof, the accumulated hydrogen **could not be outflow** in time and could only spread in all directions along the horizontal.
- The accumulated hydrogen gradually spread to the roof's edge and then into the atmosphere.

RESULTS AND DISCUSSION

Leakage angle θ=90°



t = 1s

t = 3s

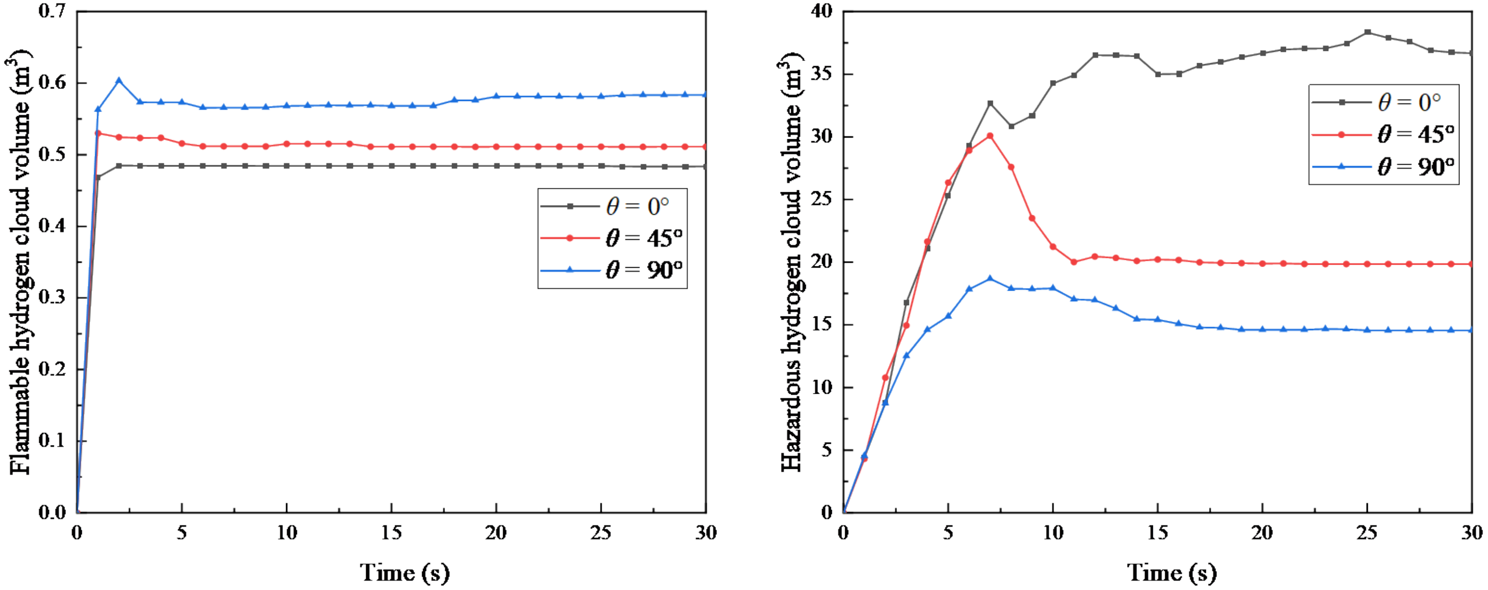
t = 5s

t = 30s

- The volume of the flammable hydrogen cloud **decreased rapidly** and remained stable.
- The vertical momentum was converted into **horizontal momentum** under the obstacle and redirection effect of the roof, and the momentum **dropped significantly**.
- The vortex formed at the end of the jet was smaller, and the hazardous hydrogen cloud volume decreased from the peak to the steady state took longer.

RESULTS AND DISCUSSION

Flammable and hazardous hydrogen cloud volumes



a. Flammable hydrogen cloud volume variation curve with time at different leakage angles

b. Hazardous hydrogen cloud volume variation curve with time at different leakage angles

- Even if the obstacle was farther away, it would significantly **hindered the diffusion of the diluted hydrogen** (vol% from 1% to 4%).
- Hydrogen would easily accumulate near the obstacle, thus **forming a large volume of hazardous hydrogen cloud**.
- At θ=45°, the volume of the hazardous hydrogen cloud continued to increase and reached its peak at approximately 7 seconds.

CONCLUSIONS

- For a hydrogen refueling station in Ningbo Zhoushan Port of China, a three-dimensional model was built.
- Closer obstacles slightly increase the accumulated flammable hydrogen cloud, while more distant obstacles significantly increase the volume of the hazardous hydrogen cloud.
- In the case of three different leakage angles, the volume of the flammable hydrogen cloud was maximum when $\vartheta=90°$, which was 18.89% more than that when $\vartheta=0°$.
- Predicting the evolution of hydrogen diffusion characteristics under obstacle structure can help improve the safety of hydrogen refueling stations.

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Thanks for your attentions!

Weiyi Cui[1, 2, 3], Liang Tong[1, 2, 4], Yupeng Yuan[1, 2, 4, 5] and Chengqing Yuan[1, 2, 4, 5]

[1] State Key Laboratory of Maritime Technology and Safety, Wuhan University of Technology, Wuhan, 430063, China.
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